

Report for JSPS – FAPESP Joint Research Workshop FY2016Date December 12 20161. Title of Workshop JSPS-FAPESP Joint Research Workshop – Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental ApproachesURL http://www.ncube.human.nagoya-u.ac.jp/mscrs2016/

2. Purpose of Workshop

Photochemistry and photobiology are important research fields from both scientific and industrial aspects. To understand various phenomena involving light-induced activations and reactions as well as photochromic systems for solar energy storage, both science and technology have been greatly developed so far. However, even now, we still often face experimental difficulties in observing the molecular behavior at local spatial and short time scales. On the other hand, recent theoretical methods can directly provide atomistic level information. Nevertheless, it is rather difficult to describe potential energy surfaces on excited states in studying the long-time relaxation processes even by the present super computational techniques.

Under the circumstances, the purpose of this workshop was to discuss new possible directions of collaborations among young theoretical and experimental scientists from Japan and Brazil, aiming at revealing new frontiers of photochemistry and photobiology to develop some state-of-the-art methodologies with potential applications in these research fields.

3. Period

From October 11th 2016 through October 13th 2016 (3 days)4. Venue Noyori Conference Hall, Nagoya University, Nagoya, Japan

5. Organization

(1) Cosponsors

Japan Side	Japan Society for the Promotion of Science (JSPS)
	Nagoya University
Brazil Side	São Paulo Research Foundation (FAPESP)
	University of São Paulo

(2) Coordinator

1) Japan side

Name in full Masataka NagaokaAffiliation and Position Nagoya University, Full Professor

2) Brazil side

Name in full Sylvio Roberto Accioly CanutoAffiliation and Position University of São Paulo, Full Professor

6. Program: Agenda, Topics, Related Activities (e.g., Reception, Excursion)

*** Please append the agenda and the program to this report.

7. Mentors and Participants

1) Number of Participants

	Mentors	Participants	Others *	Total
Japan side	3	20	28	51
Brazil side	3	7	0	10
Other persons	0	0	6	6
Total	6	27	34	67

*Please include the number of participants who were not supported by this program funding.

2) List

A: Mentors

Japan side

Name in full	Affiliation/ Institution	Position	Specialty
Nobuaki KOGA	Graduate School of Information Sciences, Nagoya University	Full Professor	Quantum Chemistry
Hirofumi SATO	Graduate School of Engineering, Kyoto University	Professor	Theoretical Chemistry
Jun-ya HASEGAWA	Institute for Catalysis, Hokkaido University	Professor	Photochemistry

Brazil side

name in full	Affiliation/ Institution	Position	Specialty
Rogério, CUSTODIO	Institute of Chemistry, University of Campinas	Full Professor	Theoretical Chemistry
Herbert, GEORG	Institute of Physics, Federal University of Goiás	Professor	QM/MM Simulations
Kaline, COUTINHO	Institute of Physics, University of São Paulo	Professor	QM/MM Simulations

B: Participants

*** Please append the last version of participants list (Form 3) to this report form. ***

8. Please describe the achievements of the workshop.

We planned the Japan-Brazil (JB) Bilateral Workshop with the purpose of sharing the latest information of studies related to chemical reaction systems and biological environment involving photoexcitation and emission phenomena by using techniques of the computational and experimental science. The workshop was composed by three main topics: (1)“QM/MM Methods: Applications, Current Limitation and New Challenges”, (2) “Experimental Methods on Physical Chemistry and their Connections with Theoretical Methods and Computer Simulations” and (3) “State-of-the-Art on Photochemistry and Photobiology: From Understanding DNA Damage by Radiation to Developing New Materials”. Furthermore, we arranged the time for free discussion of current problems of both theoretical and experimental techniques, and in addition, we held a session to consider and discuss the collaborative possibility of experimentalist and theoretical researchers from Brazil and Japan.

Through the three-day workshop, we had intense and fruitful discussions and exchange of information among young scientists who are working on the elucidation of physicochemical phenomena in atomistic level by theoretical and experimental technique. In this sense, we can say the workshop completely fulfilled its main purpose. In addition, it became a reliable foundation to contribute to a deep understanding of various light-induced phenomena in the future.

As for the concrete actions for future collaboration, by now, Nagoya University and University of São Paulo have already an agreement for exchange programs and international collaborations, making possible the exchange of master and PhD students as well as the mutual visits of Professors and Post-Doctoral fellows. Based on the mutual understanding in the workshop, we expect that the international exchange between the two countries becomes more active in the future.

In addition, concerning the training of young researchers in the future, we made a mailing list that includes all participants from both countries. By using this mailing list, several kind of useful information can be shared, such as opportunities for exchange students, fellowships for postdoctoral and young researchers, international meeting and conferences, etc. All those information will facilitate and strengthen the possibility of collaboration in near future. The clarification of physicochemical phenomena in an atomistic level depends on collaborative work among experts in both, experimental and theoretical fields, given the challenging complexity involved. By sharing and discussing the current understanding of the field in these topics, and the present challenges that have to be faced, the collaborative research among young scientists will certainly be promoted.

平成28年度若手研究者ワークショップ 参加者リスト

平成 28年 10月 14日

ワークショップ名: Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental Approaches

1. 日本側参加者リスト

No	姓	名	所属機関・部局	職名	所属国名 ¹⁾	備考 ²⁾
No	Family Name	Name	Affiliation	Job Title	Country ¹⁾	Note ²⁾
1	長岡	正隆	名古屋大学・大学院情報科学研究科	教授	日本	*
1	Nagaoka	Masataka	Graduate School of Information Science, Nagoya University	Professor	Japan	
2	古賀	伸明	名古屋大学・大学院情報科学研究科	教授	日本	*
2	Koga	Nobuaki	Graduate School of Information Science, Nagoya University	Professor	Japan	
3	佐藤	啓文	京都大学・大学院工学研究科	教授	日本	*
3	Satou	Hirofumi	Graduate School of Engineering, Kyoto University	Professor	Japan	
4	長谷川	淳也	北海道大学・触媒科学研究所	教授	日本	*
4	Hasegawa	Junya	Institute for Catalysis, Hokkaido University	Professor	Japan	
5	ビスタファ	カルロス	名古屋大学・大学院情報科学研究科	博士研究員	日本	*
5	Bistafa	Carlos	Graduate School of Information Science, Nagoya University	PostDoctoral Research Fellow	Japan	
6	北村	勇吉	名古屋大学・大学院情報科学研究科	博士研究員	日本	*
6	Kitamura	Yukichi	Graduate School of Information Science, Nagoya University	PostDoctoral Research Fellow	Japan	
7	高柳	昌芳	名古屋大学・大学院情報科学研究科	特任助教	日本	*
7	Takayanagi	Masayoshi	Graduate School of Information Science, Nagoya University	Project Assistant Professor	Japan	
8	竹中	規雄	名古屋大学・大学院情報科学研究科	特任助教	日本	*
8	Takenaka	Norio	Graduate School of Information Science, Nagoya University	Project Assistant Professor	Japan	
9	横川	大輔	名古屋大学・大学院理学研究科	特任准教授	日本	*
9	Yokogawa	Daisuke	Graduate School of Science, Nagoya University	Associate Professor	Japan	
10	チェン	ユエ	北海道大学・触媒科学研究所	博士研究員	日本	*
10	Chen	Yue	Institute for Catalysis, Hokkaido University	PostDoctoral Research Fellow	Japan	
11	原 渕	祐	北海道大学・大学院理学研究院	博士研究員	日本	*
11	Harabuchi	Yu	Faculty of Science, Hokkaido University	PostDoctoral Research Fellow	Japan	
12	中山	哲	北海道大学・触媒科学研究所	准教授	日本	*
12	Nakayama	Akira	Institute for Catalysis, Hokkaido University	Associate Professor	Japan	
13	ラタンサク	マヌサーダ	北海道大学・触媒科学研究所	博士研究員	日本	*
13	Ratanasak	Manussada	Institute for Catalysis, Hokkaido University	PostDoctoral Research Fellow	Japan	
14	斉田	謙一郎	北海道大学・大学院理学研究院	特任助教	日本	*
14	Saita	Kenichiro	Faculty of Science, Hokkaido University	Project Assistant Professor	Japan	

15	ハッサニアンアレイ	ハディ	京都大学・大学院理学研究科	博士研究員	日本	*
15	Hassanian Arefi	Hadi	Graduate School of Science, Kyoto University	PostDoctoral Research Fellow	Japan	
16	山崎	祥平	弘前大学・大学院理工学研究科	助教	日本	*
16	Yamazaki	Shohei	Graduate School of Science and Technology, Hirosaki University	Assistant Professor	Japan	
17	城塚	達也	東北大学・大学院理学部研究科	研究員	日本	*
17	Joutsuka	Tatsuya	Graduate School of Science, Tohoku University	Researcher	Japan	
18	バラドウワジ	プラディーブ	東京大学・化学システム工学科	博士研究員	日本	*
18	Varadwaj	Pradeep	Chemical System Engineering, The University of Tokyo	PostDoctoral Research Fellow	Japan	
19	北	幸海	横浜市立大学 大学院生命ナノシステム科学研究科	准教授	日本	*
19	Kita	Yukiumi	Graduate School of Nanobioscience, Yokohama City University	Associate Professor	Japan	
20	川口	一朋	金沢大学・理工研究域 数物科学系	助教	日本	*
20	Kawaguchi	Kazutomo	Institute of Science and Engineering, Kanazawa University	Assistant Professor	Japan	
21	本林	健太	名古屋工業大学・フロンティア研究院	助教	日本	*
21	Motobayashi	Kenta	Frontier Research Institute, Nagoya Institute of Technology	Assistant Professor	Japan	
22	赤瀬	大	広島大学・大学院理学研究科	博士研究員	日本	*
22	Akase	Dai	Graduate School of Science, Hiroshima University	PostDoctoral Research Fellow	Japan	
23	水上	渉	九州大学・総合理工学研究院	助教	日本	*
23	Mizukami	Wataru	Faculty of Engineering Science, Kyushu Hiroshima University	Assistant Professor	Japan	
24	東	雅大	琉球大学・海洋自然科学科	助教	日本	*
24	Higashi	Masahiro	Department of Chemistry, Biology and Marine Science, University of the Ryukyus	Assistant Professor	Japan	
25	菱川	明栄	名古屋大学・大学院理学研究科	教授	日本	
25	Hishikawa	Akiyoshi	Graduate School of Science, Nagoya University	Professor	Japan	
26	稲垣	泰一	名古屋大学・大学院情報科学研究科	博士研究員	日本	
26	Inagaki	Taichi	Graduate School of Information Science, Nagoya University	PostDoctoral Research Fellow	Japan	
27	伊藤	克浩	名古屋大学・大学院情報科学研究科	学生	日本	
27	Ito	Katsuhiro	Graduate School of Information Science, Nagoya University	Student	Japan	
28	井内	哲	名古屋大学・大学院情報科学研究科	助教	日本	
28	Iuchi	Satoru	Graduate School of Information Science, Nagoya University	Assistant Professor	Japan	
29	ウップラ	プルショッタム	名古屋大学・大学院情報科学研究科	博士研究員	日本	
29	Uppla	Purushotham	Graduate School of Information Science, Nagoya University	PostDoctoral Research Fellow	Japan	
30	栗崎	以久男	名古屋大学・大学院情報科学研究科	博士研究員	日本	
30	Kurisaki	Ikuo	Graduate School of Information Science, Nagoya University	PostDoctoral Research Fellow	Japan	
31	鈴木	雄一	名古屋大学・大学院情報科学研究科	学生	日本	
31	Suzuki	Yuichi	Graduate School of Information Science, Nagoya University	Student	Japan	

32	藤江	拓哉	名古屋大学・大学院情報科学研究科	学生	日本	
32	Fujie	Takuya	Graduate School of Information Science, Nagoya University	Student	Japan	
33	前田	猛	名古屋大学・大学院情報科学研究科	学生	日本	
33	Maeda	Takeshi	Graduate School of Information Science, Nagoya University	Student	Japan	
34	松本	健太郎	名古屋大学・大学院情報科学研究科	学生	日本	
34	Matsumoto	Kentaro	Graduate School of Information Science, Nagoya University	Student	Japan	
35	山口	毅	名古屋大学・大学院工学研究科	助教	日本	
35	Yamaguchi	Tsuyoshi	Graduate School of Engineering, Nagoya University	Assistant Professor	Japan	
36	吉田	久美	名古屋大学・情報文化学部	教授	日本	
36	Yoshida	Kumi	School of Informatics and Sciences, Nagoya University	Professor	Japan	
37	笠原	健人	京都大学・大学院工学研究科	学生	日本	
37	Kasahara	Kento	Graduate School of Engineering, Kyoto University	Student	Japan	
38	松三	勇介	京都大学・大学院工学研究科	学生	日本	
38	Matsumi	Yusuke	Graduate School of Engineering, Kyoto University	Student	Japan	
39	シシュキン	マキシム	京都大学・実験と理論計算科学のインターフェイスによる触媒・電池の元素戦略研究拠点	研究員	日本	
39	Shishkin	Maxim	ESICB, Kyoto University	Researcher	Japan	
40	シャンカー	サドハンシュ	京都大学・大学院工学研究科	博士研究員	日本	
40	Shanker	Sudhanshu	Graduate School of Science, Kyoto University	PostDoctoral Research Fellow	Japan	
41	山本	武志	京都大学・大学院理学研究科	助教	日本	
41	Yamamoto	Takeshi	Graduate School of Science, Kyoto University	Assistant Professor	Japan	
42	炭竈	享司	福井大学・医学部	助教	日本	
42	Sumikama	Takashi	Faculty of Medical Sciences, University of Fukui	Assistant Professor	Japan	
43	大西	拓	三重大学・大学院工学研究科	助教	日本	
43	Onishi	Taku	Department of Chemistry for Materials and CUTE, Mie University	Assistant Professor	Japan	
44	川嶋	裕介	大阪大学・大学院薬学研究科	学生	日本	
44	Kawashima	Yusuke	Graduate School and School of Pharmaceutical Science	Student	Japan	
45	中田	真秀	理化学研究所 情報基盤センター	技師	日本	
45	Nakata	Masahide	Advanced Center for Computing and Communication	Engineer	Japan	
46	張	賀東	名古屋大学 大学院情報科学研究科	准教授	日本	
46	Chan	Futon	Graduate School of Information Science, Nagoya University	Associate Professor	Japan	
47	安田	耕二	名古屋大学 未来材料・システム研究科	准教授	日本	
47	Ysuda	Koji	Institute of Materials and Systems for Sustainability	Associate Professor	Japan	
48	吉田	悠一郎	京都大学・大学院工学研究科	学生	日本	
48	Yoshida	Yuichiro	Graduate School of Engineering, Kyoto University	Student	Japan	

49	稲井	直人	名古屋大学大学院理学研究科(物質理学専攻 量子化学グループ)	学生	日本	
49	Inai	Naoto	Graduate School of Science, Nagoya University	Student	Japan	
50	中瀧	翔太	名古屋大学大学院理学研究科(物質理学専攻 量子化学グループ)	学生	日本	
50	Nakataki	Shota	Graduate School of Science, Nagoya University	Student	Japan	
51	須田	佳代	名古屋大学大学院理学研究科(物質理学専攻 量子化学グループ)	学生	日本	
51	Suda	Kayo	Graduate School of Science, Nagoya University	Student	Japan	
52	三澤	奈々	東京大学大学院 工学系研究科 化学生命工学専攻	学生	日本	
52	Misawa	Nana	School of Engineering, the University of Tokyo	Student	Japan	

1) 参加者が所属する機関の所在国を記入してください

2) 本ワークショップ経費にて参加される方については、備考欄に「*」を記入してください。

List of Participants for JSPS-FAPESP Joint Research Workshop 2016

Date: Oct. 14th 2016

Workshop Title: Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental Approaches

2. List of participants on the Brazilian side

No	Family Name	Name	Affiliation	Job Title	Country ¹⁾	Note ²⁾
1	ACCIOLY CANUTO	Sylvio Roberto	University of São Paulo	Professor	Brazil	*
2	CUSTODIO	Rogério	University of Campinas	Professor	Brazil	*
3	GEORG	Herbert	Federal University of Goiás	Professor	Brazil	*
4	COUTINHO	Kaline	University of São Paulo	Professor	Brazil	*
5	BARBOSA FERREIRA	Marcos Antonio	Federal University of São Carlos	Professor	Brazil	*
6	HOMEM DE MELLO	Paula	Federal University of ABC	Professor	Brazil	*
7	MARTÍNEZ	Leandro	University of Campinas	Professor	Brazil	*
8	PEREIRA DOS SANTOS	Diego	University of Campinas	Professor	Brazil	*
9	SCHWAB	Ricardo Samuel	Federal University of São Carlos	Professor	Brazil	*
10	SPARVOLI DE MEDEIROS	Marina	Federal University of ABC	Professor	Brazil	*
11	TROIANO FELICIANO	Gustavo	São Paulo State University	Professor	Brazil	*

¹⁾ Please write a country of affiliated institution.

²⁾ Please put "*" in this section when FAPESP/JSPS pays his/her expenses.

平成28年度若手研究者ワークショップ 参加者リスト

平成 28年 10月 14日

ワークショップ名: Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental Approaches

3. その他の国からの参加者リスト

No	姓	名	所属機関・部局	職名	所属国名 ¹⁾	備考 ²⁾
No	Family Name	Name	Affiliation	Job Title	Country ¹⁾	Note ²⁾
1	アギユラー	マニエルアソゲル	エストレマドゥーラ 大学	教授	スペイン	
1	Aguilar	Manuel Angel	University of Extremadura	Professor	Spain	
2	ドメーネ	カルメン	キングスカレッジ ロンドン	教授	英国	
2	Domene	Carmen	King's College London	Professor	UK	
3	リー	サンヨブ	ソウル大学校	教授	韓国	
3	Lee	Sangyoub	Seoul National University	Professor	South Korea	
4	ナヴァホ	マリアエレナマルチン	エストレマドゥーラ 大学	教授	スペイン	
4	Navarro	Maria Elena Martin	University of Extremadura	Professor	Spain	
5	ロベール	ヴァンサン	ストラスブール大学	教授	フランス	
5	Robert	Vincent	University of Strasbourg	Professor	France	
6	ヴェララウシ	サージ	ストラスブール大学	教授	フランス	
6	Vela Llausí	Sergi	University of Strasbourg	Professor	France	

JSPS-FAPESP Joint Research Workshop Questionnaire for the Participants

Workshop Title Overseas Challenges in Photochemical and Photobiological Sciences via Computational and Experimental Approaches

**Among the participants, 23 people kindly answered the questionnaire.
In the following, we summarize the results.**

Part 1

Please let us know how you evaluate this workshop so that we can improve our workshops in the future.
Circle the letter from A to E that matches closest your opinion.

The letters stand for the following:

A = strongly agree **B** = agree **C** = neutral **D** = disagree **E** = completely disagree

	A	B	C	D	E
Organization of the workshop					
-The time allotted to each part of the program was appropriate	16	5	1	0	0
-The lecture and laboratory components were effectively linked	12	7	3	1	0
-The size of the classes was optimal	14	6	3	0	0
Lectures					
-Sufficient time was allocated for the lectures	15	5	3	0	0
-The lectures were useful in my research (interesting, stimulating and practical)	11	8	4	0	0
-The level of the lectures relative to my educational background and experience was optimal	7	12	3	0	0
Discussions					
-Sufficient time was allocated for the discussions	10	8	4	1	0
-The discussions were useful in my research (interesting, stimulating and practical)	8	11	4	0	0
Lecturers					
-Lecturers gave equal treatment to all the participants	13	7	2	1	0
-Lecturers respected the ideas, opinions and comments of the participants	13	9	1	0	0

Overall

-I found my participation in the workshop to be meaningful	11	9	2	0	0
-I was able to create and expand working networks with other researchers by participating in the workshop	10	7	5	0	0

Part 2

Please write your comments.

-The most successful aspect of this workshop:

Several participants praised the level of the talks as also as the opportunity to meet researchers from a different scientific community.

In addition, several have pointed out that the workshop was an excellent opportunity for young researchers present their works and construct collaborative networks.

-The least successful aspect of this workshop (if possible, suggestion for improvement):

Some of the participants pointed out that they would like to have even more time for free discussion about the topics and possible collaborations. However, based on the format of the workshop and the number of attendants, this would be only possible if in future editions, the workshop had a longer duration (4 or 5 days).

-Other comments:

- none -

